6-Quinolinamine, N,N,2-trimethyl-92-99-9 | DTXSID6059075

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 3.77e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.87e-01

Confidence level: 3.68e-01

Nearest Neighbors from the Training Set

Image not found

Bis(ethylxanthogen) Measured: 1.14e-05 Predicted: 4.06e-05

Image not found

Heptachlor epoxide Measured: 5.14e-07 Predicted: 3.52e-07

Image not found

5-methyl-1-phenylpyrrolidin-2-

one

Measured: 1.43e-01 Predicted: 3.13e-01